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NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 JAN 17 Pre-1988 INPI data added to MARPAT
NEWS 4 FEB 21 STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5 FEB 22 The IPC thesaurus added to additional patent databases on STN
NEWS 6 FEB 22 Updates in EPFULL; IPC 8 enhancements added
NEWS 7 FEB 27 New STN AnaVist pricing effective March 1, 2006
NEWS 8 MAR 03 Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9 MAR 22 EMBASE is now updated on a daily basis
NEWS 10 APR 03 New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 11 APR 03 Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 12 APR 04 STN AnaVist \$500 visualization usage credit offered
NEWS 13 APR 12 LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14 APR 12 Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 15 APR 12 Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 16 MAY 10 CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 17 MAY 11 KOREAPAT updates resume
NEWS 18 MAY 19 Derwent World Patents Index to be reloaded and enhanced

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT <http://download.cas.org/express/v8.0-Discover/>

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8
NEWS X25 X.25 communication option no longer available after June 2006

Enter NEWS followed by the item number or name to see news on that specific topic.

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*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

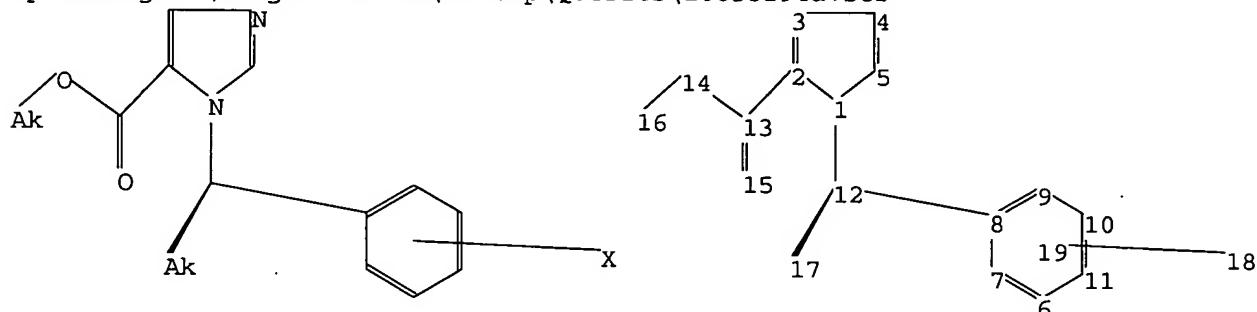
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10635294a.str



chain nodes :

12 13 14 15 16 17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-12 2-13 8-12 12-17 13-14 13-15 14-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-5 1-12 3-4 4-5 12-17 13-14 13-15 14-16

exact bonds :

2-3 2-13 8-12

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems :

containing 1 : 6 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
 19:CLASS

05/24/2006 10635294c.trn

Stereo Bonds:

17-12 (Single Wedge).

Stereo Chiral Centers:

12 (Parity=Don't Care)

Stereo RSS Sets:

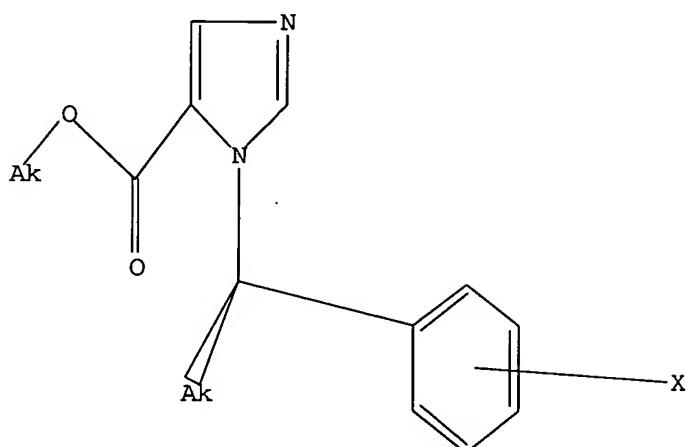
Type=Relative (Default). 1 Nodes= 12

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 14:55:34 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 468 TO ITERATE

100.0% PROCESSED 468 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 8063 TO 10657

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s 11 sss full

FULL SEARCH INITIATED 14:55:40 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 9425 TO ITERATE

100.0% PROCESSED 9425 ITERATIONS

26 ANSWERS

05/24/2006 10635294c.trn

SEARCH TIME: 00.00.01

L3 26 SEA SSS FUL L1

=> FIL HCAPLUS	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	166.94	167.15

FILE 'HCAPLUS' ENTERED AT 14:55:46 ON 24 MAY 2006
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FILE COVERS 1907 - 24 May 2006 VOL 144 ISS 22
FILE LAST UPDATED: 23 May 2006 (20060523/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 8 L3

=> s 14 and radioactive halogen
173123 RADIOACTIVE
28 RADIOACTIVES
173132 RADIOACTIVE
(RADIOACTIVE OR RADIOACTIVES)
106628 HALOGEN
21560 HALOGENS
117523 HALOGEN
(HALOGEN OR HALOGENS)
78 RADIOACTIVE HALOGEN
(RADIOACTIVE(W) HALOGEN)
1 L4 AND RADIOACTIVE HALOGEN

=> s 14 and radioactive
173123 RADIOACTIVE
28 RADIOACTIVES
173132 RADIOACTIVE
(RADIOACTIVE OR RADIOACTIVES)
L6 2 L4 AND RADIOACTIVE

=> d 15 ibib abs hitstr tot

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:123220 HCAPLUS
 DOCUMENT NUMBER: 142:198079
 TITLE: Preparation of radiolabeled 1-(phenylethyl)imidazole-5-carboxylic acid ester derivatives
 INVENTOR(S): Zolle, Ilse; Hammerschmidt, Friedrich
 PATENT ASSIGNEE(S): Austria
 SOURCE: U.S. Pat. Appl. Publ., 15 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005033060	A1	20050210	US 2003-635294 US 2003-635294	20030806 20030806
PRIORITY APPLN. INFO.:				
OTHER SOURCE(S):	CASREACT 142:198079; MARPAT 142:198079			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Halogenated carboxylic ester derivs. of phenylethylimidazole (I) [R1 = linear or branched C1-4 alkyl which is optionally substituted with a halogen selected from the groups consisting of F, Cl, I or Br; R2 = C1-2 alkyl; X = a nonradioactive or a radioactive halogen] or (II) [X = a nonradioactive or radioactive halogen selected from the group consisting of I, Br, and F; X = a radioactive halogen selected from the group consisting of 123I, 124I, 131I, 76Br, 82Br or 18F] are prepared via coupling of (S)-secondary alc. (III) (R2, X = same as above) with imidazolecarboxylate ester (IV) (R1 = same as above). Radio-halogenated forms of these compds. are ideally suited for positron-imaging of the adrenal glands, as it is known that these compds. demonstrate a selective and high rate of accumulation in the adrenals. The method of preparing these derivs. proceeds by the conversion of a stable, non-radioactive intermediate having trialkylstannyll leaving groups (V) [R1, R2 = same as above; L = an alkylstannyll group selected from the group consisting of trimethylstannyll, triethylstannyll, tri-n-propylstannyll and tri-n-butylstannyll] and (VI) (R1, R2 = same as above). These intermediates are efficiently converted to the corresponding halogenated forms by substitution of the trialkylstannyll group with the halogen or radiohalogen. Thus, 4-iodoacetophenone was reduced by DIBAH in toluene/Et2O at -78° to give 86% 1-(4-iodophenyl)ethanol which was esterified by chloroacetic anhydride in the presence of pyridine in CH2Cl2 at 0° for 2 h to give 91% 1-(4-iodophenyl)ethyl chloroacetate (VII). VII underwent enzymic hydrolysis in the presence of lipase SAM II in a mixture of tert-Bu Me ether and phosphate buffer at 0° for 2 h while keeping pH at 7.0 by adding 0.5 N aqueous NaOH solution to give 43% (R)-1-(4-iodophenyl)ethanol (98% ee) and 44% (S)-1-(4-iodophenyl)ethyl chloroacetate (>98% ee) (VIII). VIII was coupled with Me 3H-imidazole-4-carboxylate using triphenylphosphine and di(tert-butyl) azocarboxylate in THF at -30° to 0° over 2.5 h to give 67% (R)-(+)-Me 3-[1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate (99% ee) which was refluxed with hexamethyltin in toluene at 135° for 17 h to give 96% (R)-(+)-Me 3-[1-[4-(trimethylstannyll)phenyl]ethyl]-3H-imidazole-4-carboxylate (IX).

IX (30 μ g) was reacted with [^{131}I]iodide in 10-20 μ L 0.05 N aqueous NaOH solution, 15 μ L aqueous chloramine-T solution (1 mg/mL), and 6 μ L 1 N aqueous HCl solution at room temperature for 1 min to give (R)-(+)-Me 3-[1-(4-[^{131}I]iodophenyl)ethyl]-3H-imidazole-4-carboxylate (^{131}I -MTO), i.e. II (R1 = R2 = Me, X = ^{131}I).

IT 813466-09-0P

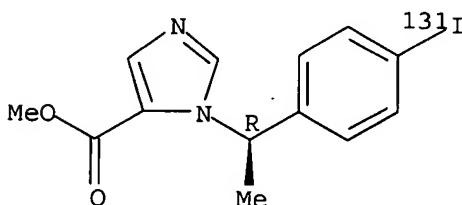
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-09-0 HCPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo- ^{131}I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 813466-05-6P, (R)-(+)-Methyl 3-[1-(4-Iodophenyl)ethyl]-3H-imidazole-4-carboxylate

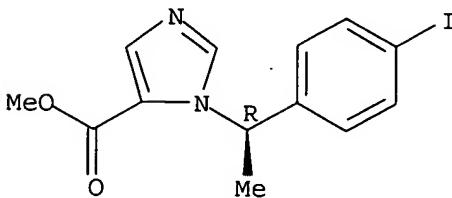
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-05-6 HCPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



=> d 16 ibib abs hitstr tot

L6 ANSWER 1 OF 2 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:123220 HCPLUS

DOCUMENT NUMBER: 142:198079

TITLE: Preparation of radiolabeled 1-(phenylethyl)imidazole-5-carboxylic acid ester derivatives

INVENTOR(S): Zolle, Ilse; Hammerschmidt, Friedrich

PATENT ASSIGNEE(S): Austria

SOURCE: U.S. Pat. Appl. Publ., 15 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005033060	A1	20050210	US 2003-635294 US 2003-635294	20030806 20030806
PRIORITY APPLN. INFO.:			CASREACT 142:198079; MARPAT 142:198079	
OTHER SOURCE(S):				
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Halogenated carboxylic ester derivs. of phenylethylimidazole (I) [R1 = linear or branched C1-4 alkyl which is optionally substituted with a halogen selected from the groups consisting of F, Cl, I or Br; R2 = C1-2 alkyl; X = a nonradioactive or a radioactive halogen] or (II) [X = a nonradioactive or radioactive halogen selected from the group consisting of I, Br, and F; X = a radioactive halogen selected from the group consisting of 123I, 124I, 131I, 76Br, 82Br or 18F] are prepared via coupling of (S)-secondary alc. (III) (R2, X = same as above) with imidazolecarboxylate ester (IV) (R1 = same as above). Radio-halogenated forms of these compds. are ideally suited for positron-imaging of the adrenal glands, as it is known that these compds. demonstrate a selective and high rate of accumulation in the adrenals. The method of preparing these derivs. proceeds by the conversion of a stable, non-radioactive intermediate having trialkylstannyll leaving groups (V) [R1, R2 = same as above; L = an alkylstannyl group selected from the group consisting of trimethylstannyl, triethylstannyl, tri-n-propylstannyl and tri-n-butylstannyl] and (VI) (R1, R2 = same as above). These intermediates are efficiently converted to the corresponding halogenated forms by substitution of the trialkylstannyl group with the halogen or radiohalogen. Thus, 4-iodoacetophenone was reduced by DIBAH in toluene/Et2O at -78° to give 86% 1-(4-iodophenyl)ethanol which was esterified by chloroacetic anhydride in the presence of pyridine in CH2Cl2 at 0° for 2 h to give 91% 1-(4-iodophenyl)ethyl chloroacetate (VII). VII underwent enzymic hydrolysis in the presence of lipase SAM II in a mixture of tert-Bu Me ether and phosphate buffer at 0° for 2 h while keeping pH at 7.0 by adding 0.5 N aqueous NaOH solution to give 43% (R)-1-(4-iodophenyl)ethanol (98% ee) and 44% (S)-1-(4-iodophenyl)ethyl chloroacetate (>98% ee) (VIII). VIII was coupled with Me 3H-imidazole-4-carboxylate using triphenylphosphine and di(tert-butyl) azocarboxylate in THF at -30° to 0° over 2 .5 h to give 67% (R)-(+)-Me 3-[1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate (99% ee) which was refluxed with hexamethyltin in toluene at 135° for 17 h to give 96% (R)-(+)-Me 3-[1-(4-(trimethylstannyl)phenyl)ethyl]-3H-imidazole-4-carboxylate (IX). IX (30 µg) was reacted with [131I]iodide in 10-20µL 0.05 N aqueous NaOH solution, 15 µL aqueous chloramine-T solution (1 mg/mL), and 6 µL 1 N aqueous HCl solution at room temperature for 1 min to give (R)-(+)-Me 3-[1-(4-[131I]iodophenyl)ethyl]-3H-imidazole-4-carboxylate (131I-MTO), i.e. II (R1 = R2 = Me, X = 131I).

IT 813466-09-0P

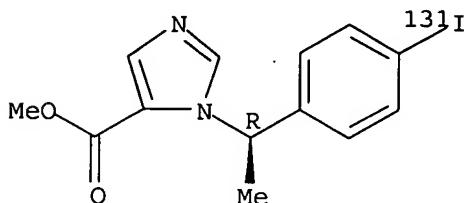
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-09-0 HCPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 813466-05-6P, (R)-(+)-Methyl 3-[(1R)-1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate

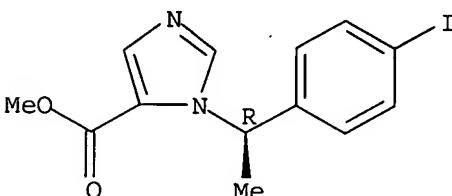
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-05-6 HCPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L6 ANSWER 2 OF 2 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:167377 HCPLUS

DOCUMENT NUMBER: 108:167377

TITLE: Synthesis of (R)-(+)-3H-etomidate

AUTHOR(S): Janssen, Cor G. M.; Thijssen, Jos B. A.; Verluyten, Willy L. M.; Heykants, Jozef J. P.

CORPORATE SOURCE: Dep. Drug Metab. Pharmacokinet., Janssen Pharm., Beerse, B-2340, Belg.

SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(8), 909-18

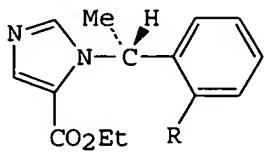
CODEN: JLCRD4; ISSN: 0362-4803

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:167377

GI



AB Etomidate, (R)-(+)-ethyl-1-(1-phenylethyl)-1H-imidazole-5-carboxylate (I, R = H) is a short-acting hypnotic. A new synthesis, featuring optical resolution on a non-radioactive precursor and introduction of the tritium label by reductive dehalogenation of I (R = Br) is described. I (R = T) was obtained at a specific activity of 3.77 Ci/mmol and a 99.9% purity.

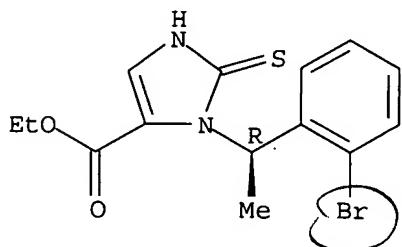
IT 112366-36-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desulfurization of, with sodium nitrite)

RN 112366-36-6 HCPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 112366-50-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 112366-50-4 HCPLUS

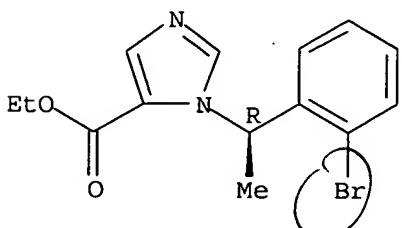
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

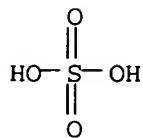
CRN 112366-49-1

CMF C14 H15 Br N2 O2

Absolute stereochemistry.

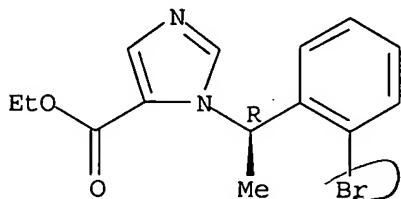


CM 2

CRN 7664-93-9
CMF H2 O4 S

IT 112366-49-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation, reductive debromination, and tritiation of)
 RN 112366-49-1 HCAPLUS
 CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester,
 (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	22.92	190.07
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

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